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Core Structure of Dissociated Dislocations in Bi_2Te_3

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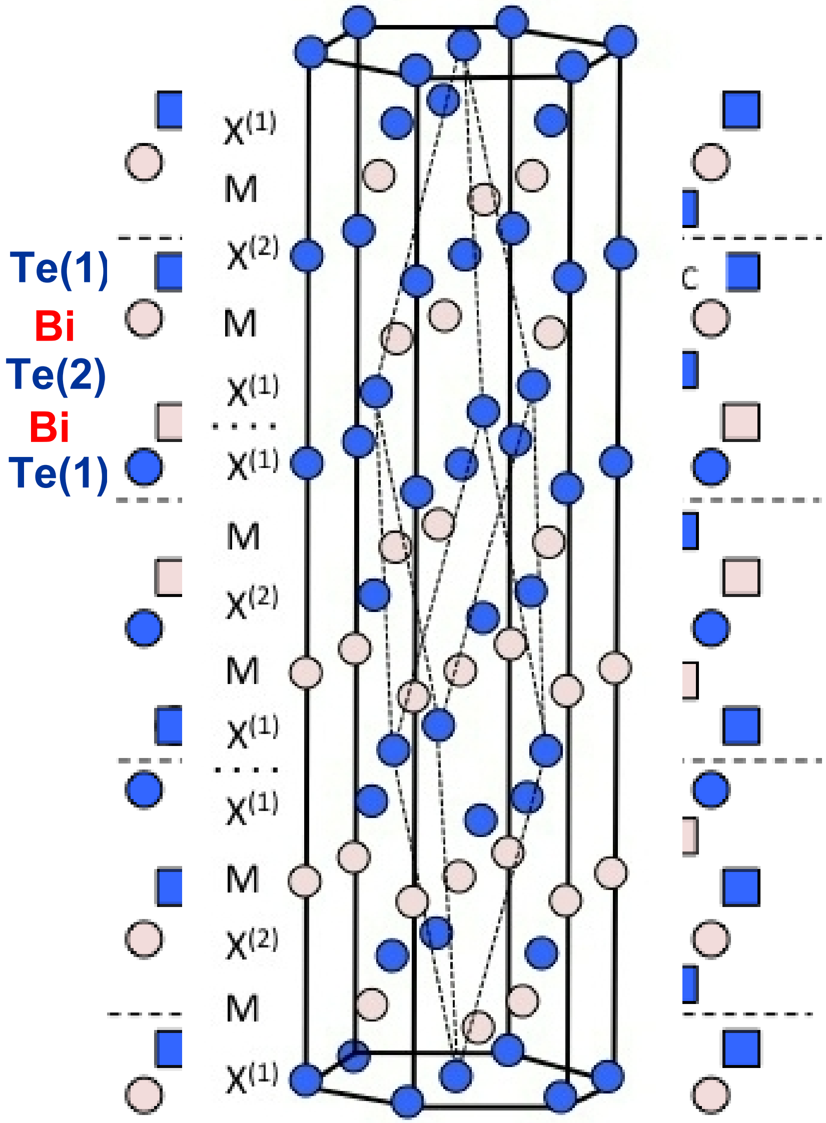
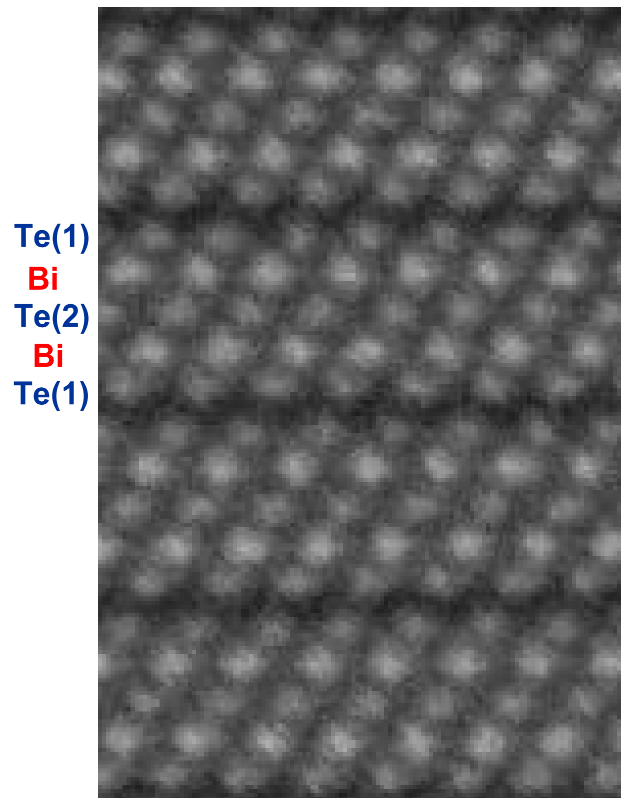
Bismuth Telluride (Bi_2Te_3): Crystal Structure



- Rhombohedral (R-3m) structure
- Based on tetradymite (Bi_2STe_2) prototype
- Three crystallographically distinct atomic sites
- $Te^{(1)}$-$Te^{(1)}$ layers: van der Waals bonding

HAADF-STEM



Bi: Z=83
Te: Z=52

Atomic number difference enables Bi and Te to be distinguished in HAADF-STEM

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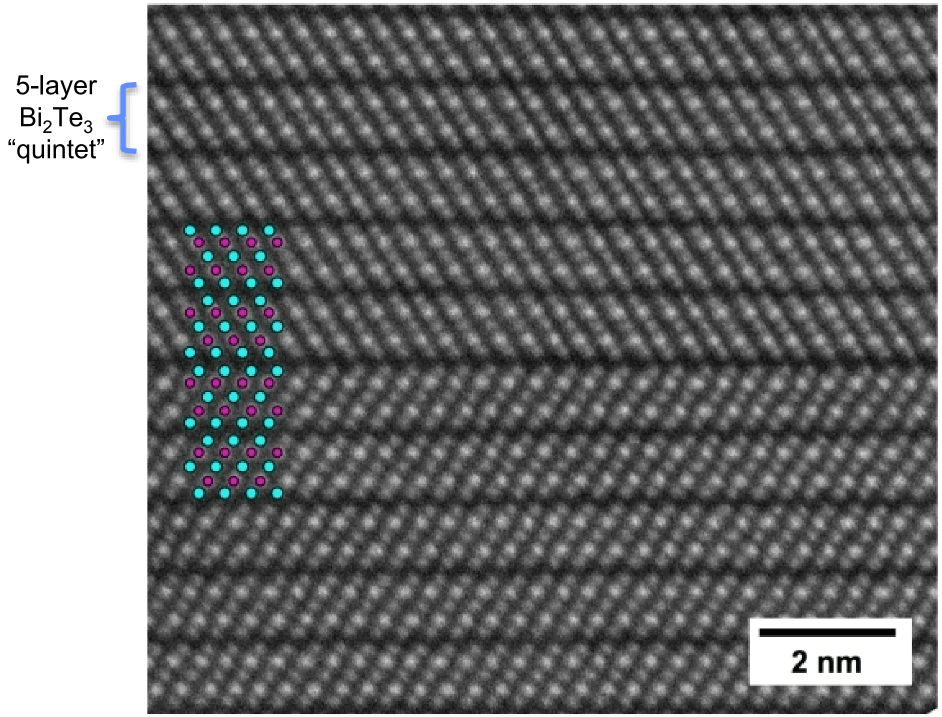
Atomic Structure of the Bi_2Te_3 Basal Twin:
Energetic preference for termination at $Te^{(1)}$ sites

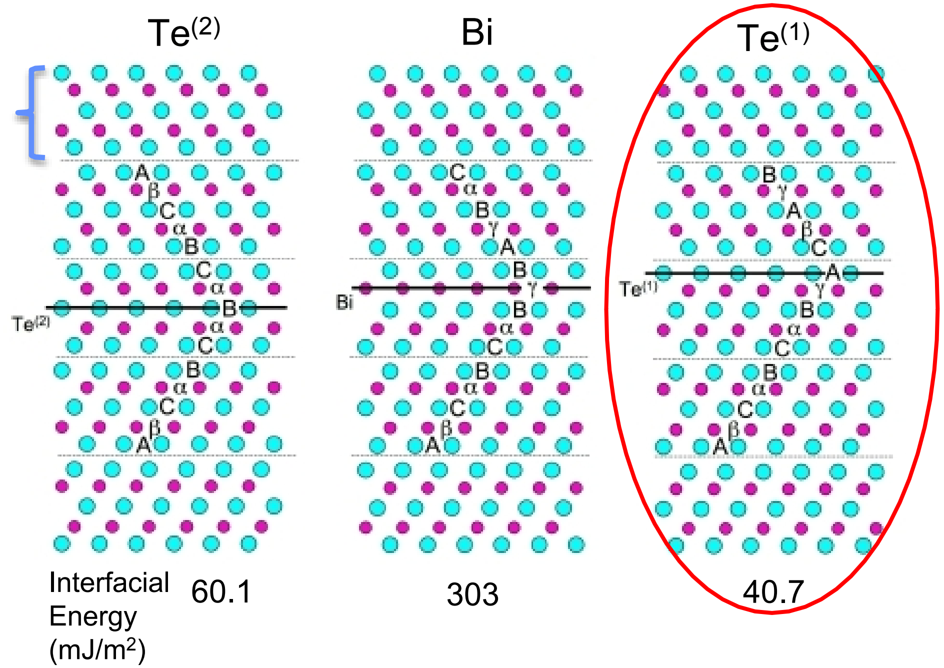
HAADF-STEM Imaging:

Twin Boundary Terminated at $Te^{(1)}$ layer



DFT Calculations:

Three Possible Compositional Terminations



D.L. Medlin, Q.M. Ramasse, C. D. Spataru, N.C. Yang, J. Appl. Phys. (2010)

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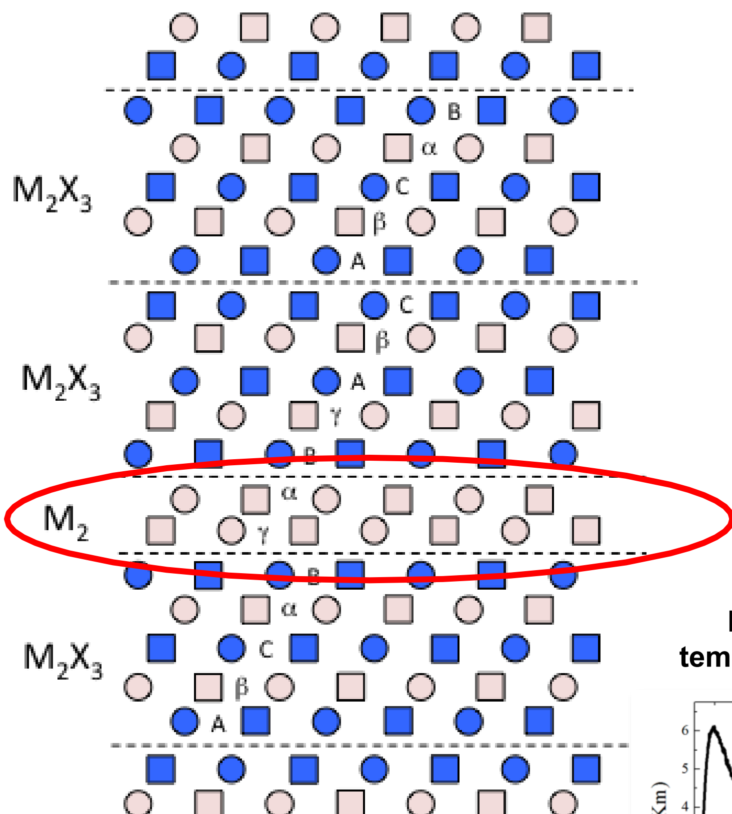
Layered structure allows flexibility in accommodating variations in composition

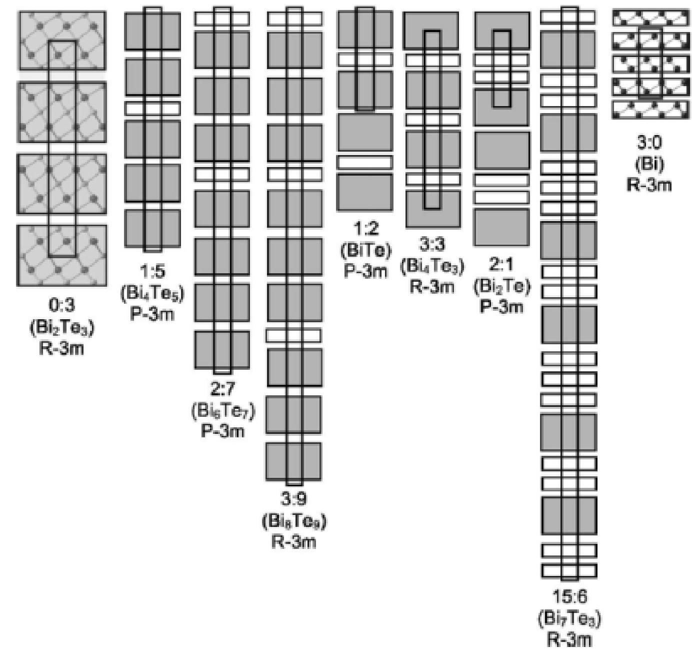
Insertion of metal bi-layers



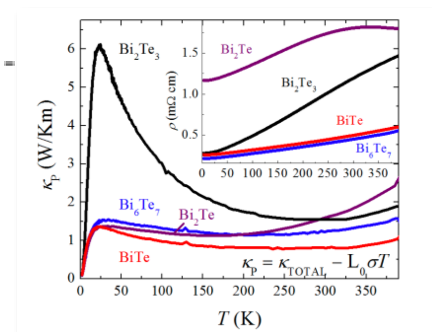
Example:
$(Bi_2)_m(Bi_2Te_3)_n$ homologous series

J.W.G. Bos, H.W. Zanderbergen, M.-H. Lee, N.P. Ong, R.J. Cava, Phys. Rev B 2007

Increasing Bismuth

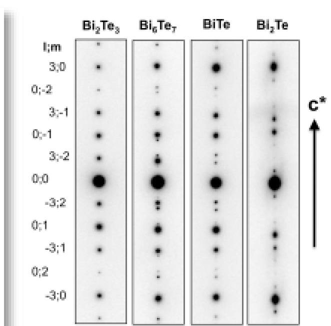


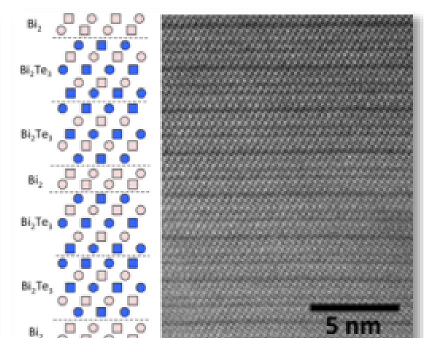
Dramatic reduction in low-temperature thermal conductivity



P. Sharma, D.Medlin, et al. PRB 83 (2011) 235209.

Electron diffraction and HRSTEM show ordering in $(Bi_2)_m(Bi_2Te_3)_n$ series

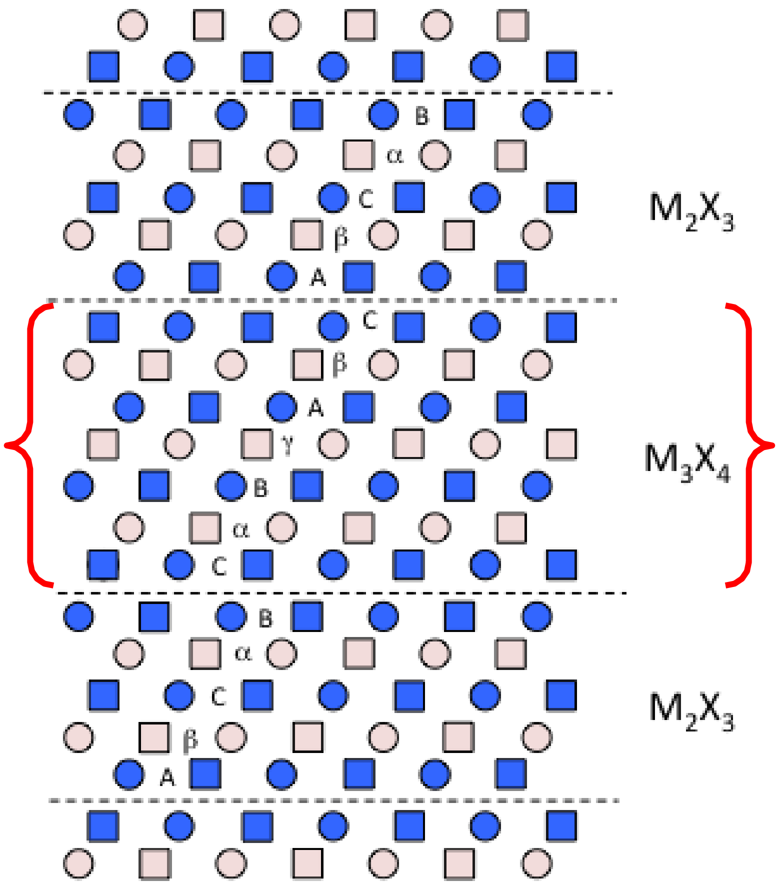




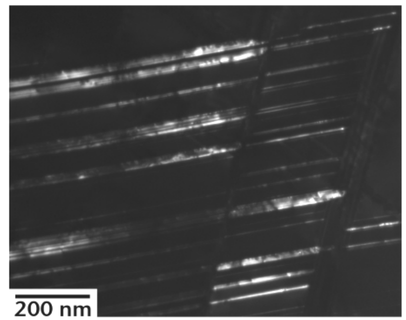
Medlin & Snyder, JOM 2013

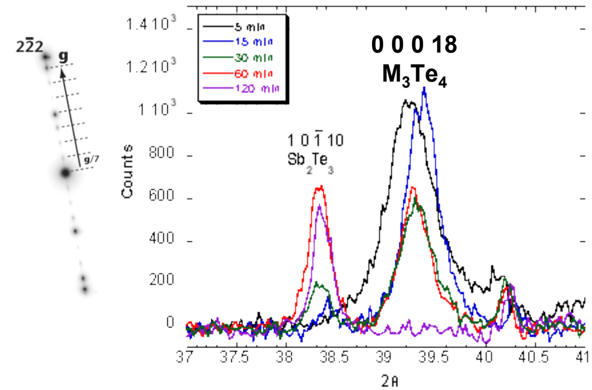
Layered structure allows flexibility in accommodating variations in composition

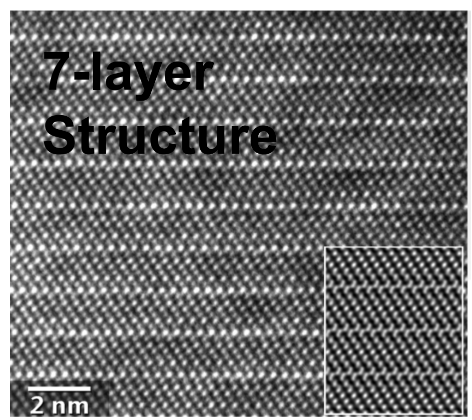
Metal rich, 7-Layer M_3X_4 fault

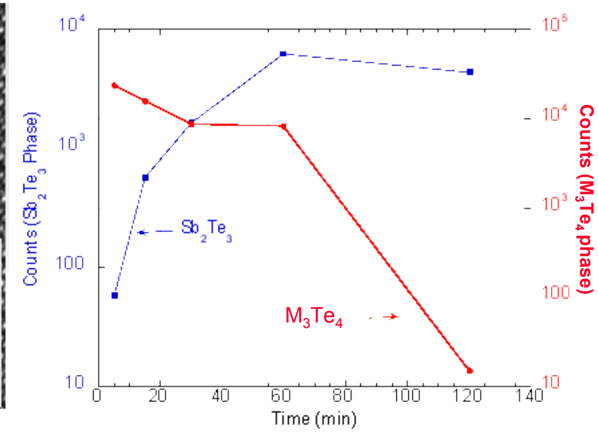


Example: $(Ag,Sb)_3Te_4$ transition phase during nucleation of Sb_2Te_3 precipitates in $AgSbTe_2$









Sharma, Sugar, & Medlin, Journal of Applied Physics (2010).
Sugar and Medlin, Journal of Materials Science (2011)

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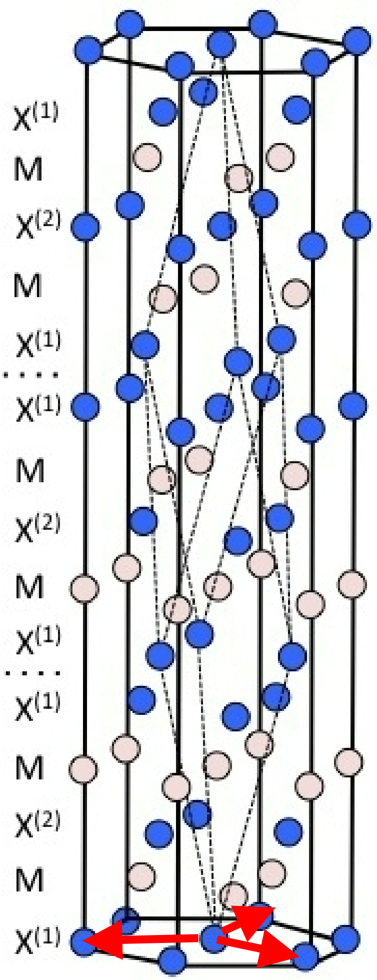
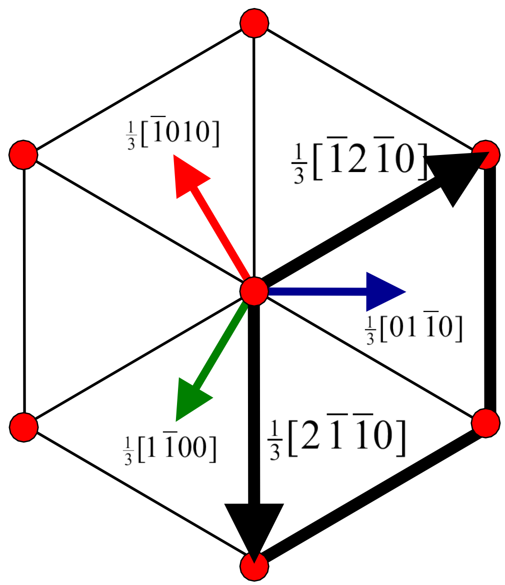
Dislocations in Bismuth Telluride

Burgers vectors lying in basal plane



Looking down on basal plane



Array of 1/3<2-1-1 0> Dislocations in Bi_2Te_3

Fig. 1. Dislocation network in Bi_2Te_3. Note that certain segments of dislocations and certain node-points have left the foil

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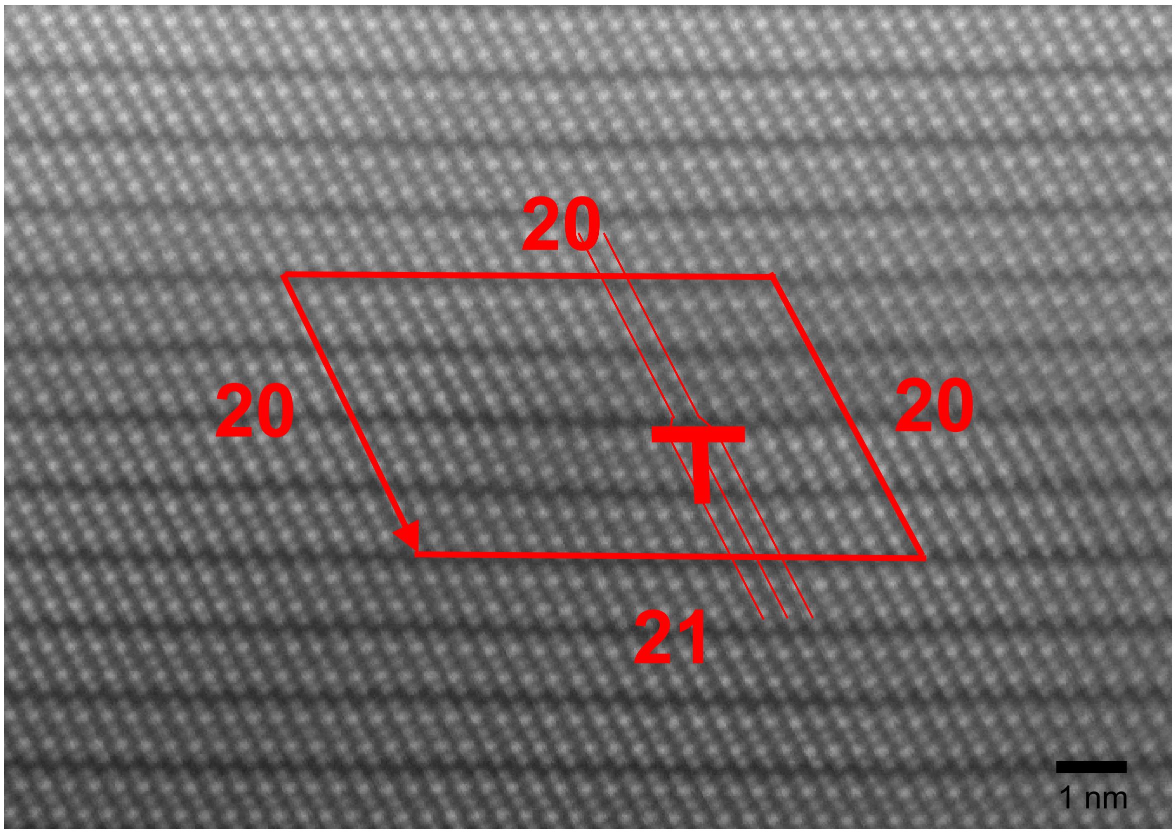
Dislocation Core structure: termination at Te$^{(1)}$-Te$^{(1)}$ layer, dissociation

5-layer Bi_2Te_3 "quintet"

[0 0 0 1]



b=1/3<2 -1 -1 0>

T 60° mixed dislocation

FEI-Titan
HAADF-STEM
300 keV

<2 -1 -1 0 > projection

Bulk Bi_2Te_3
Hot Extruded

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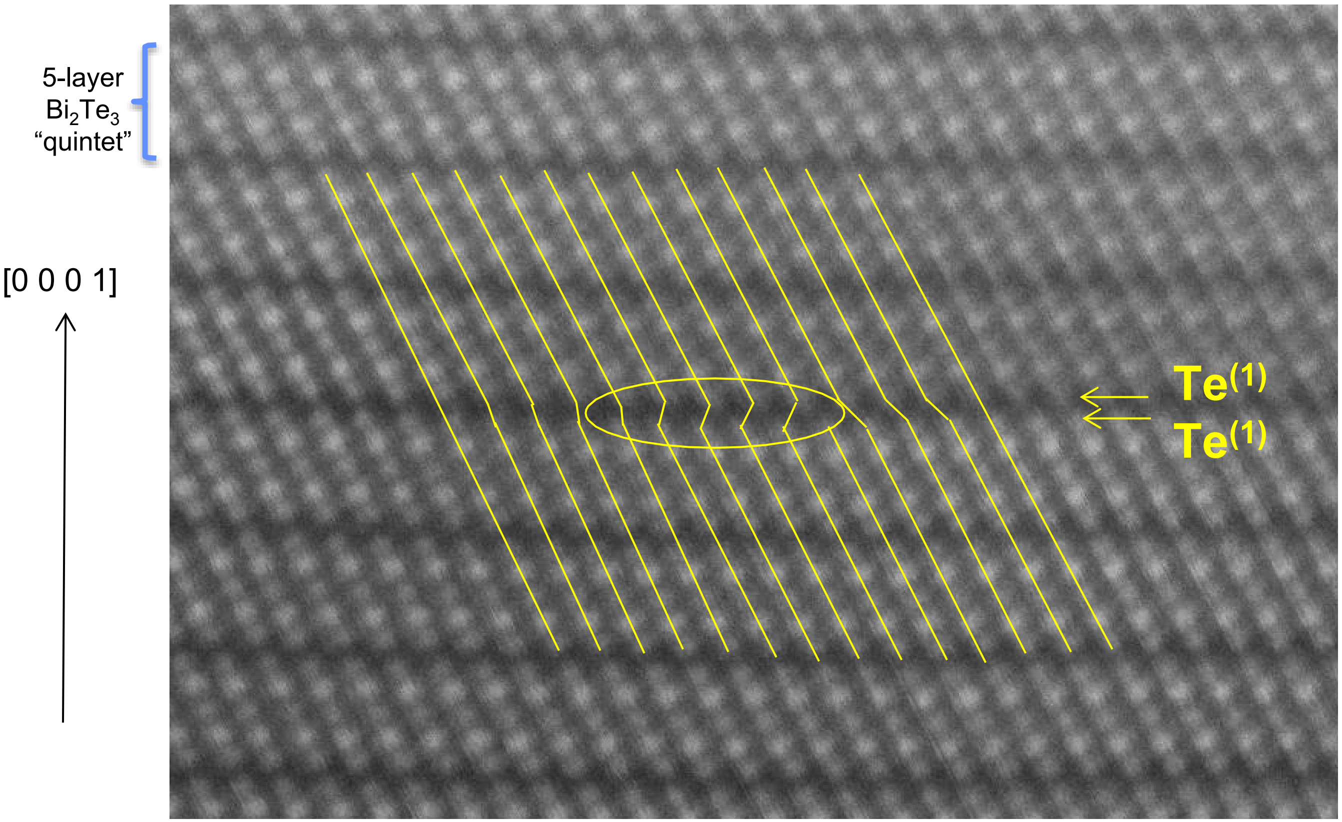
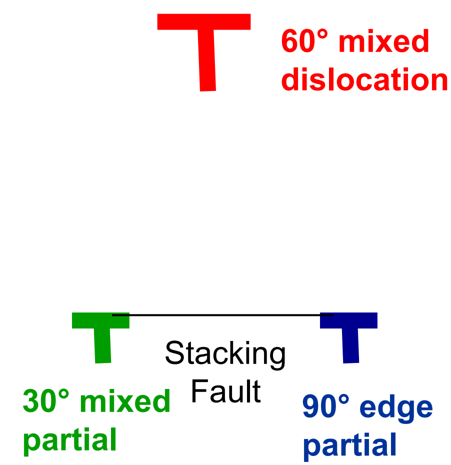
Dislocation Core structure: termination at $Te^{(1)}$-$Te^{(1)}$ layer, dissociation



b=1/3<2 -1 -1 0>



1/3<1 0 -1 0> partial dislocations.

FEI-Titan
HAADF-STEM
300 keV

Weak, van der Waals bonding likely favors dissociated dislocation core at $Te^{(1)}$-$Te^{(1)}$ layer

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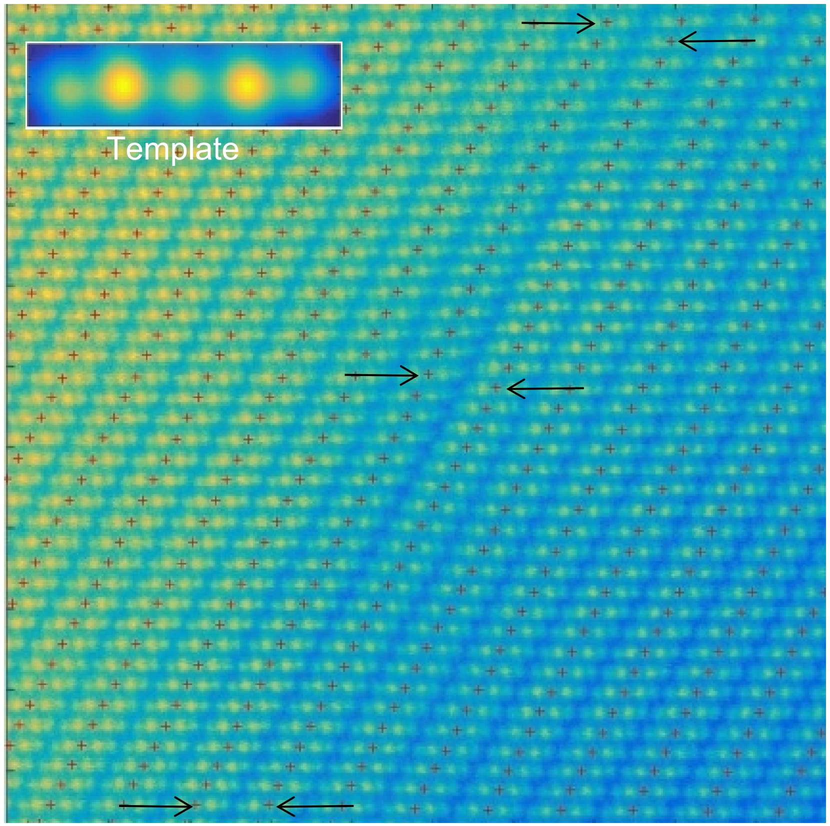
Quantify Disregistry on Slip Plane using Peierls-Nabarro Dislocation Model

Disregistry of {1 0 -1 5} planes across slip plane measured through template matching

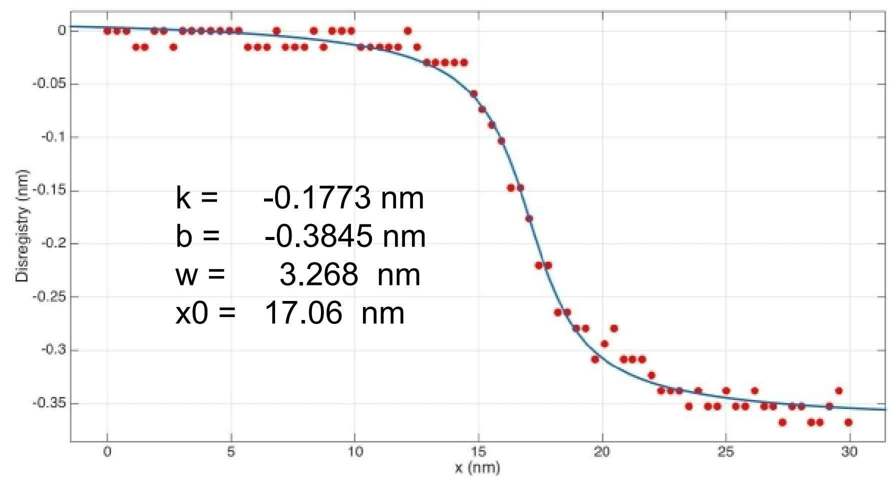


$$\underbrace{u_+ - u_-}_{\text{Disregistry}} = k + \frac{b_{edge}}{\pi}\tan^{-1}\left(\frac{x - x_0}{w/2}\right)$$

Disregistry

Burgers vector

core-width



w=3.7 nm ± 0.6 nm

6 dislocations
2-4 measurements each

μ~25.6 GPa
ν~0.26

Estimate stacking fault energy

SFE=147±23 mJ/m²

(c.f., DFT for basal twin: 41 mJ/m²)

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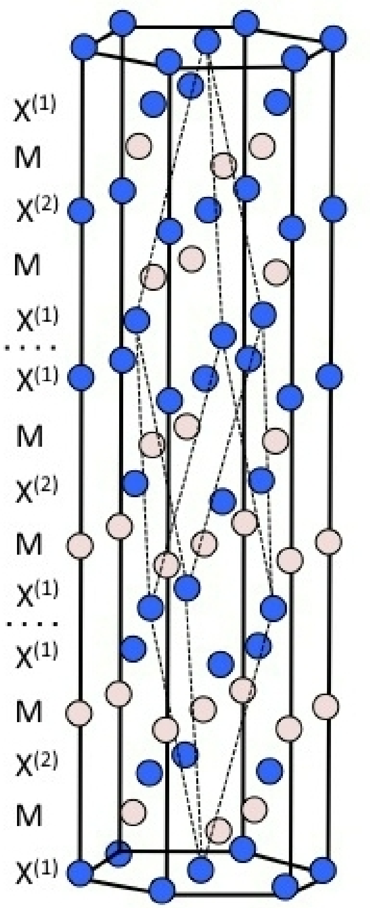
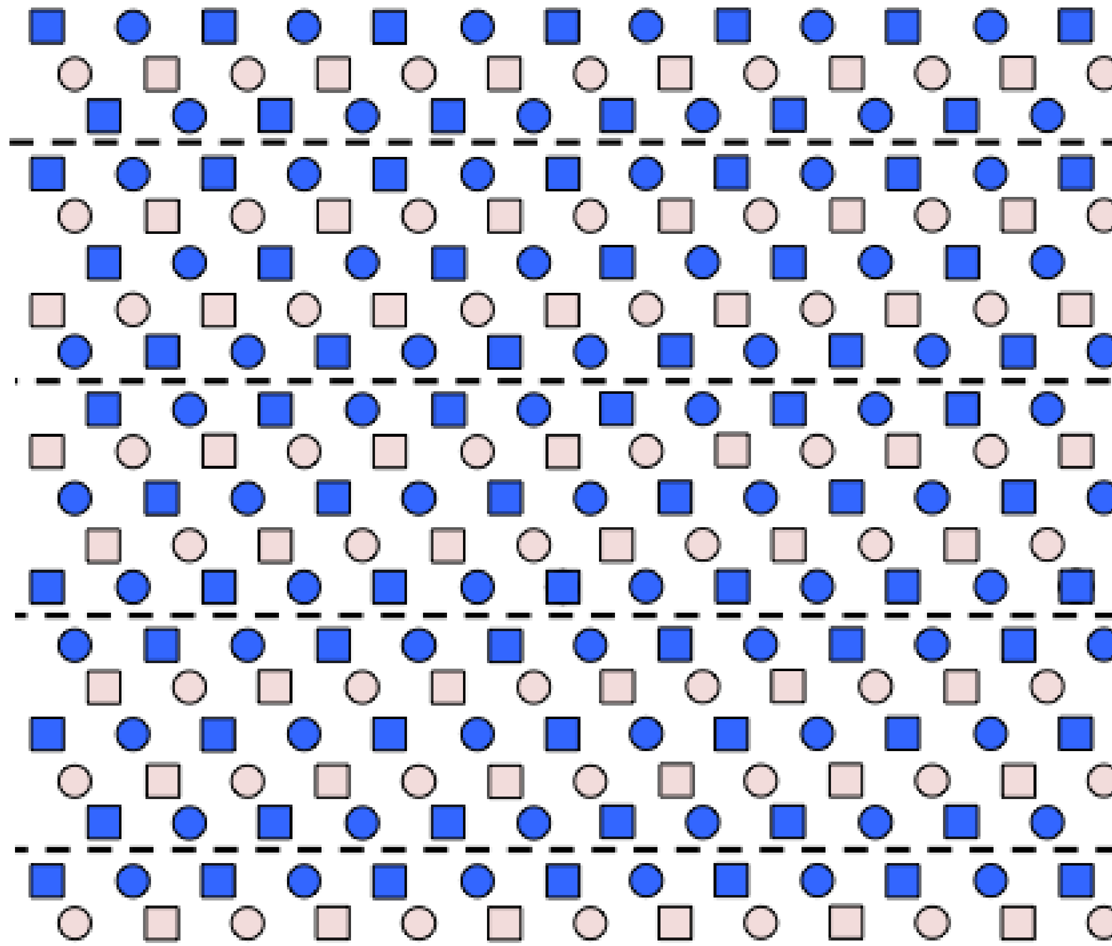
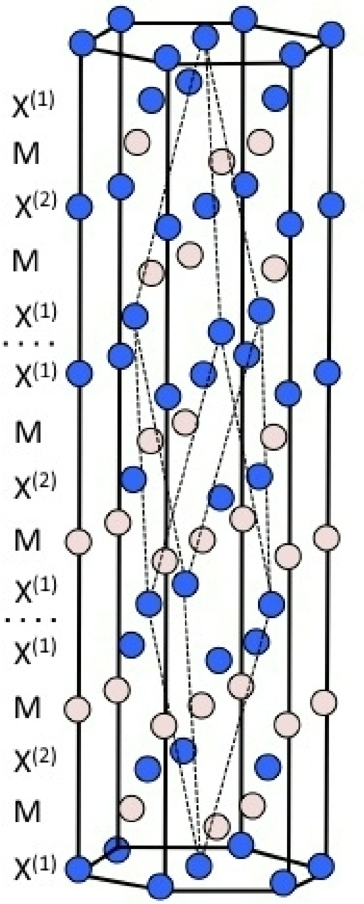
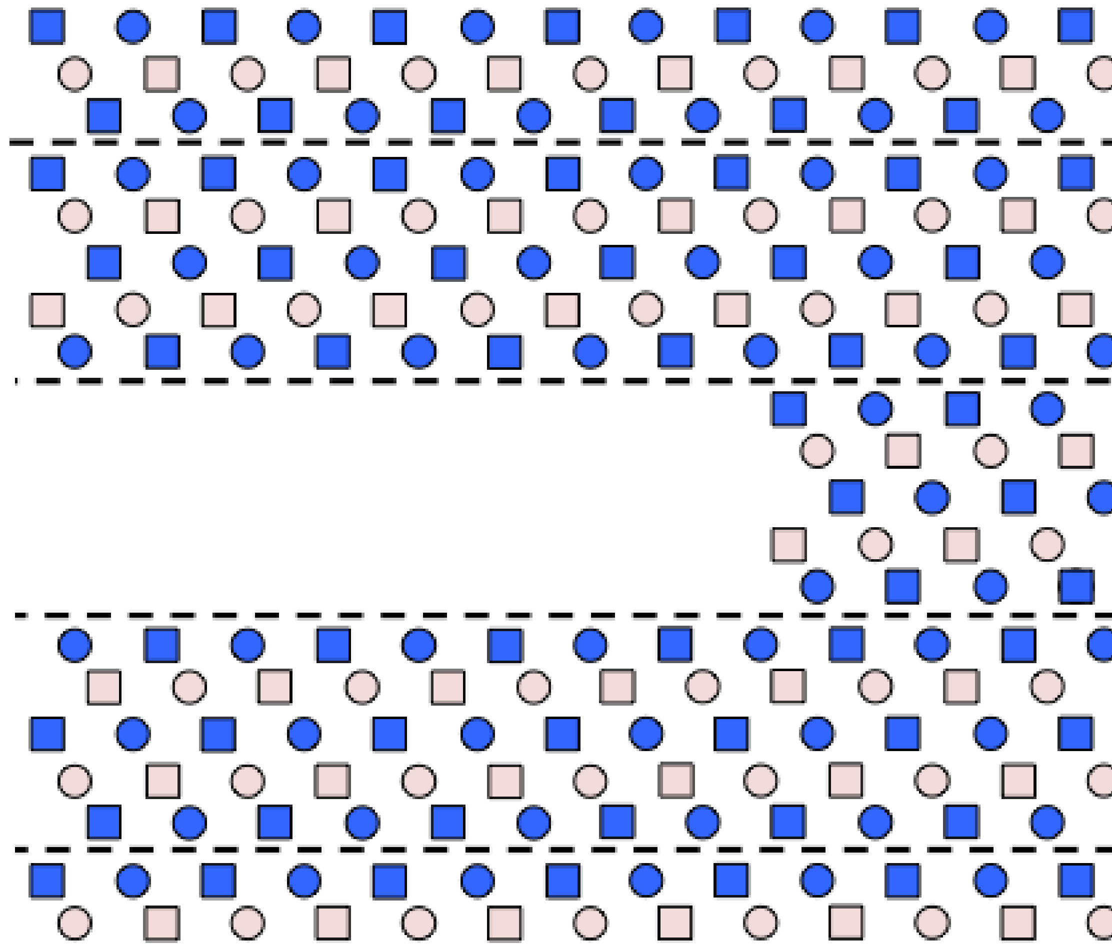
Non-basal dislocations:
What happens if we pull out a quintuple unit?





Non-basal dislocations: What happens if we pull out a quintuple unit?





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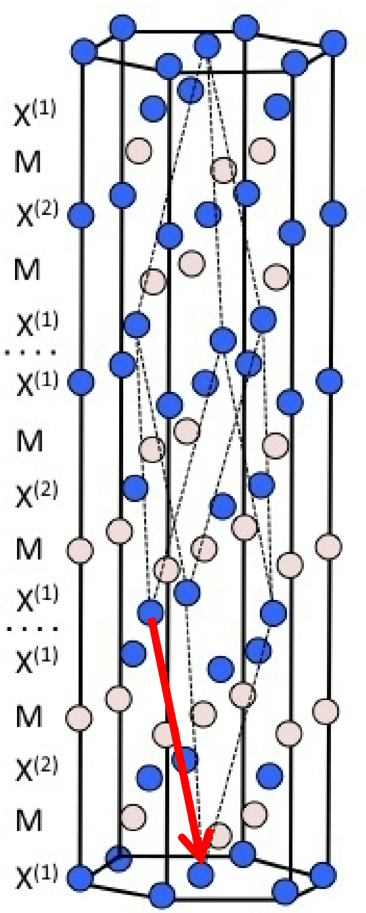
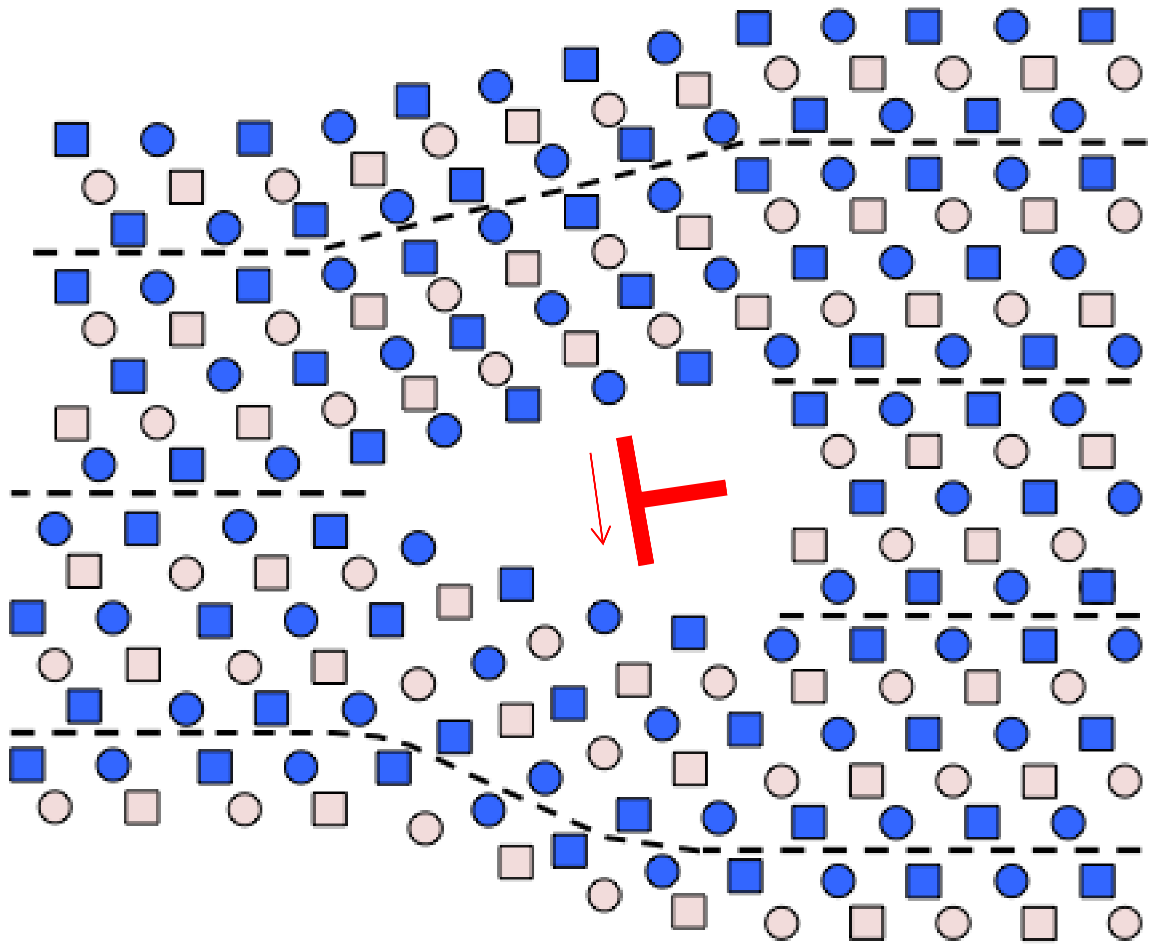
Non-basal dislocations:
What happens if we pull out a quintuple unit?





$$b = (1/3)[01\text{-}1\text{-}1]_H = [00\text{-}1]_R$$

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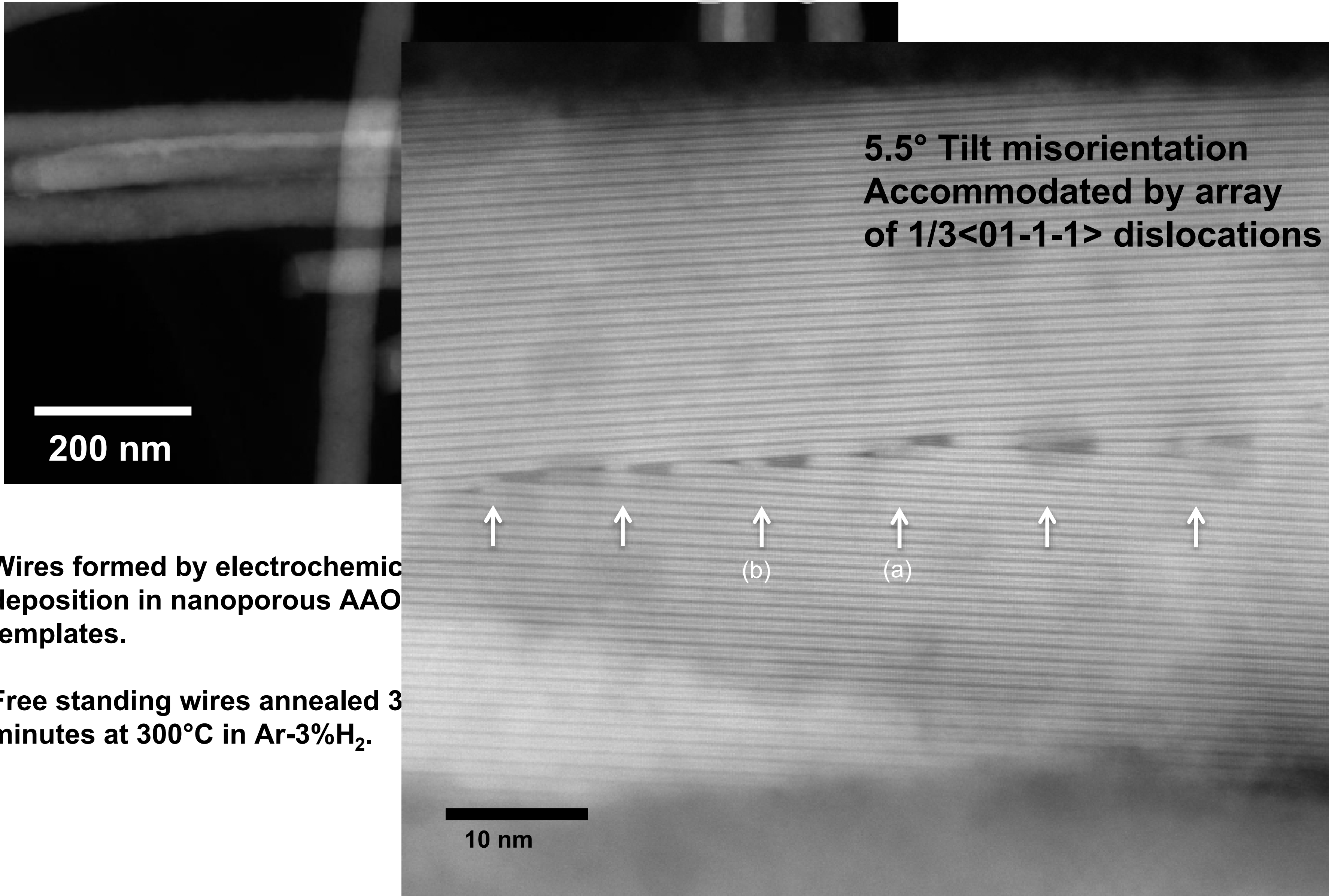
Dislocations in Bi_2Te_3 Nanowires

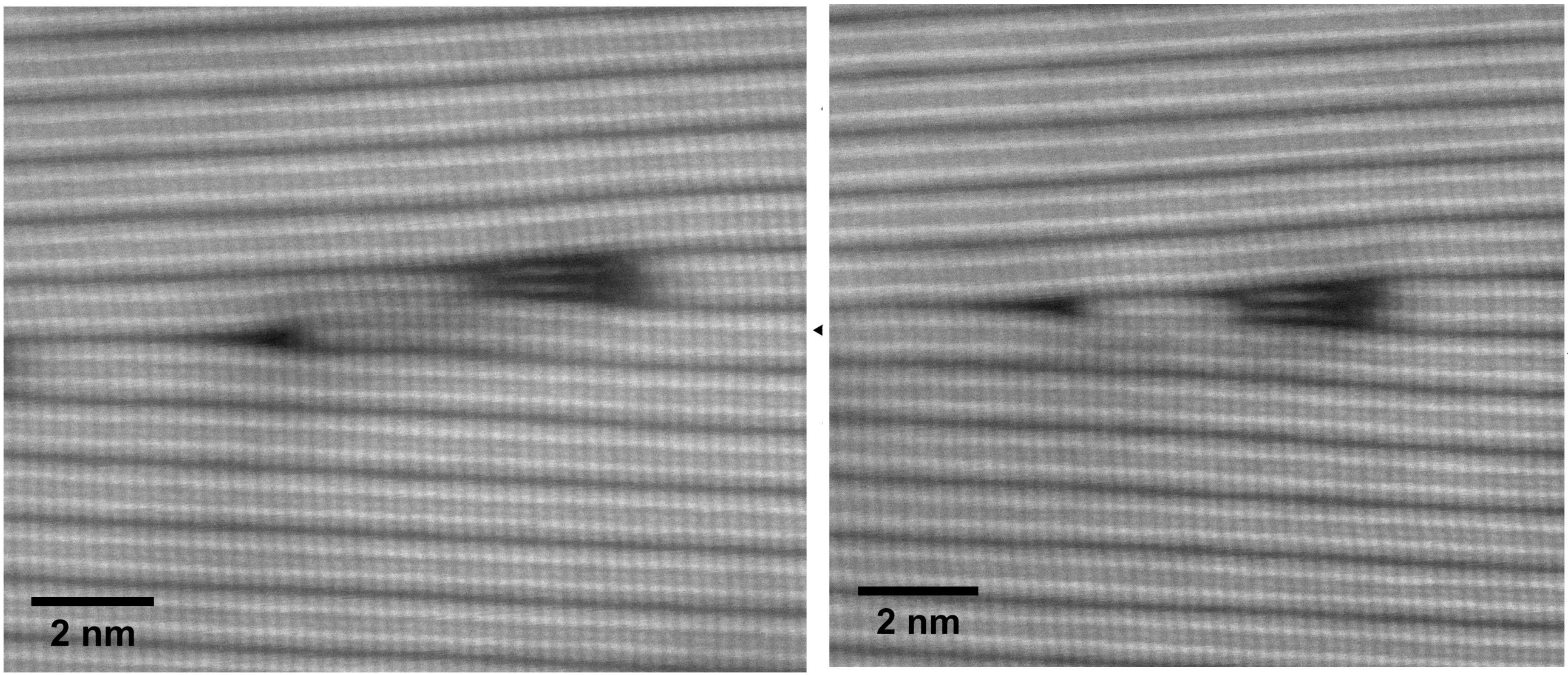


Wires formed by electrochemic deposition in nanoporous AAO templates.

Free standing wires annealed 3 minutes at 300°C in Ar-3%H_2.

Medlin, Erickson, Limmer, Yelton, Siegal, J. Mat. Sci. 2014

Dislocations have dissociated core: two configurations



<1 0 -1 0> Projection

Medlin, Erickson, Limmer, Yelton, Siegal, J. Mat. Sci. 2014

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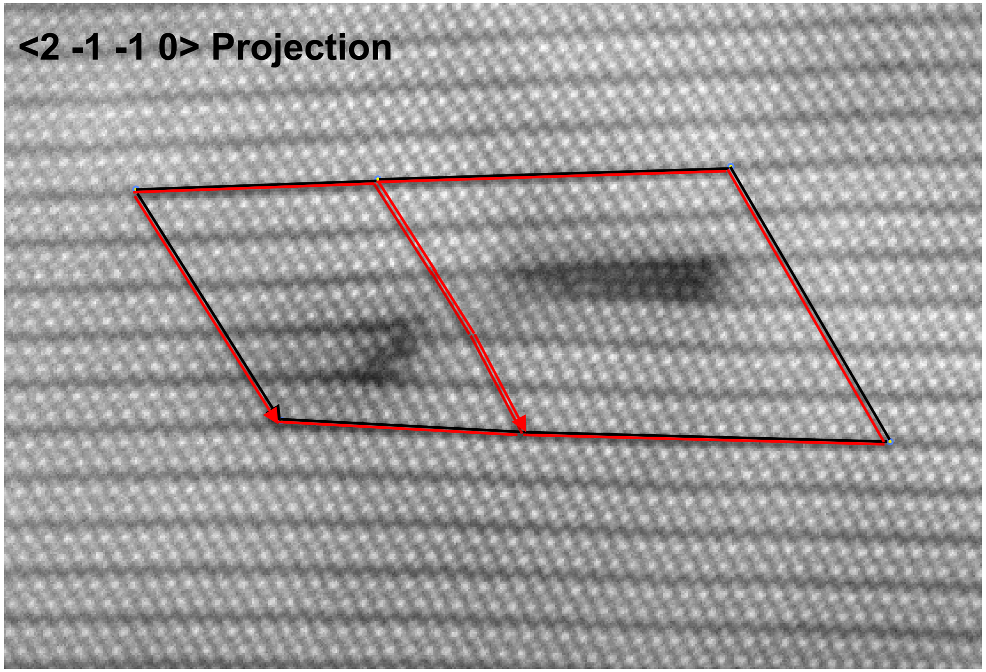
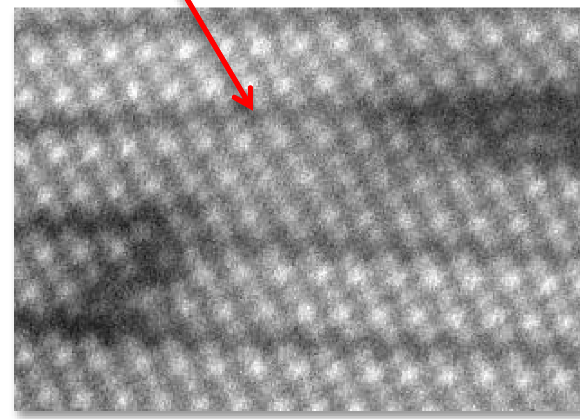
(1/3)[0 1 -1 -1] Dislocation in Bi_2Te_3:



Core structure:
Bi_3Te_4 7-layer fault



b = (1/3) [0 1 -1 -1] → (1/15) [0 5 -5 -2] + (3/15) [0 0 0 -1]

$$b^2 > b_1^2 + b_2^2$$

$$109.8 \text{ Å}^2 > 22.9 \text{ Å}^2 + 37.2 \text{ Å}^2 = 60.2 \text{ Å}^2$$

Reduced strain energy with dissociation

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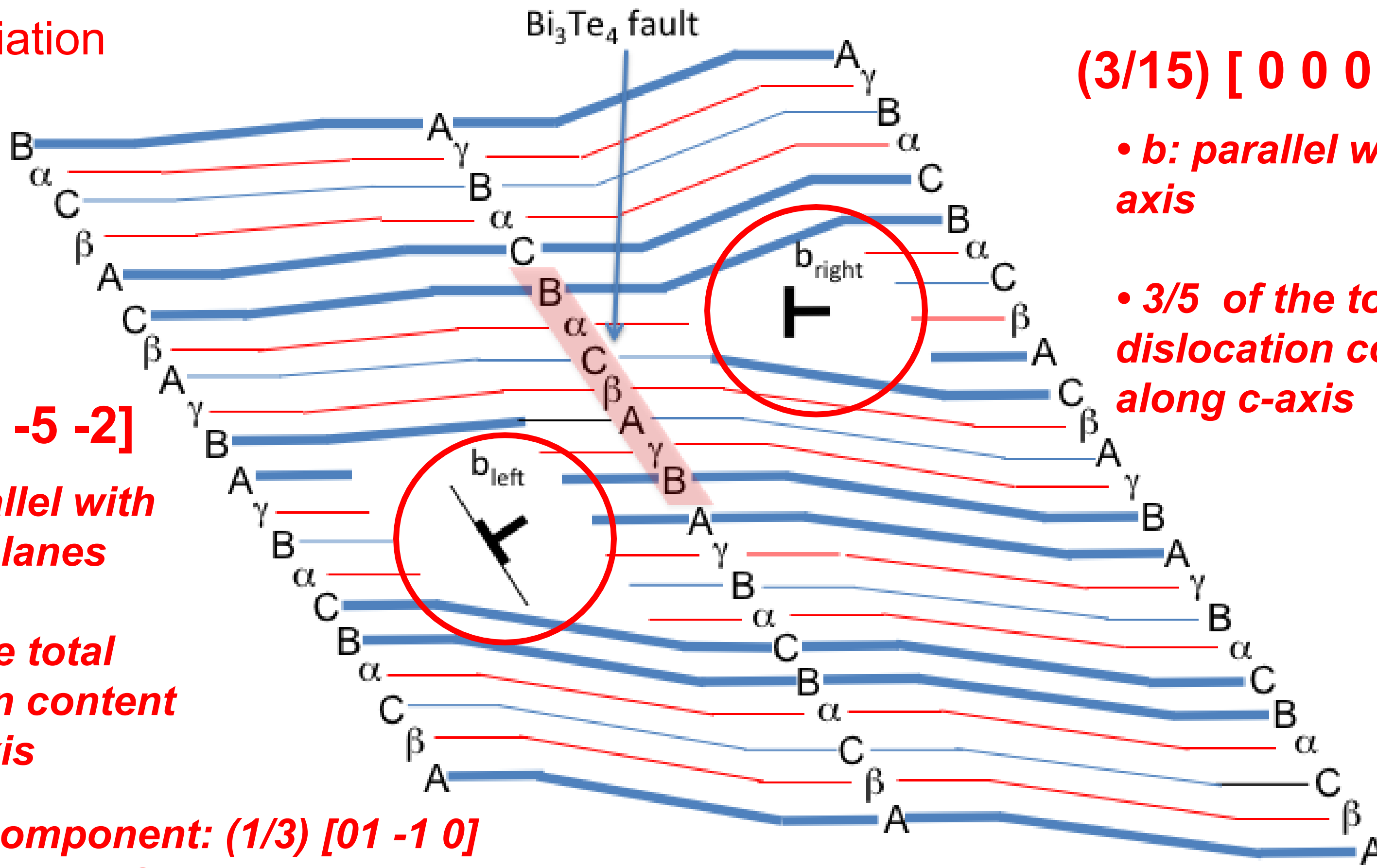
Medlin, Erickson, Limmer, Yelton, Siegal, J. Mat. Sci. 2014

7-Layer Bi_3Te_4 faults: Mechanism to accommodate Te loss during annealing

Climb dissociation



(3/15) [0 0 0 -1]

- ***b: parallel with c-axis***
- ***3/5 of the total dislocation content along c-axis***

(1/15) [0 5 -5 -2]

- ***b is parallel with (0 1 -1 5) planes***
- ***2/5 of the total dislocation content along c-axis***

Horizontal component: (1/3) [01 -1 0]

- ***analogous to Shockley partial.***
- ***avoids fault in stacking resulting from additional 2 planes at Bi_3Te_4 fault***

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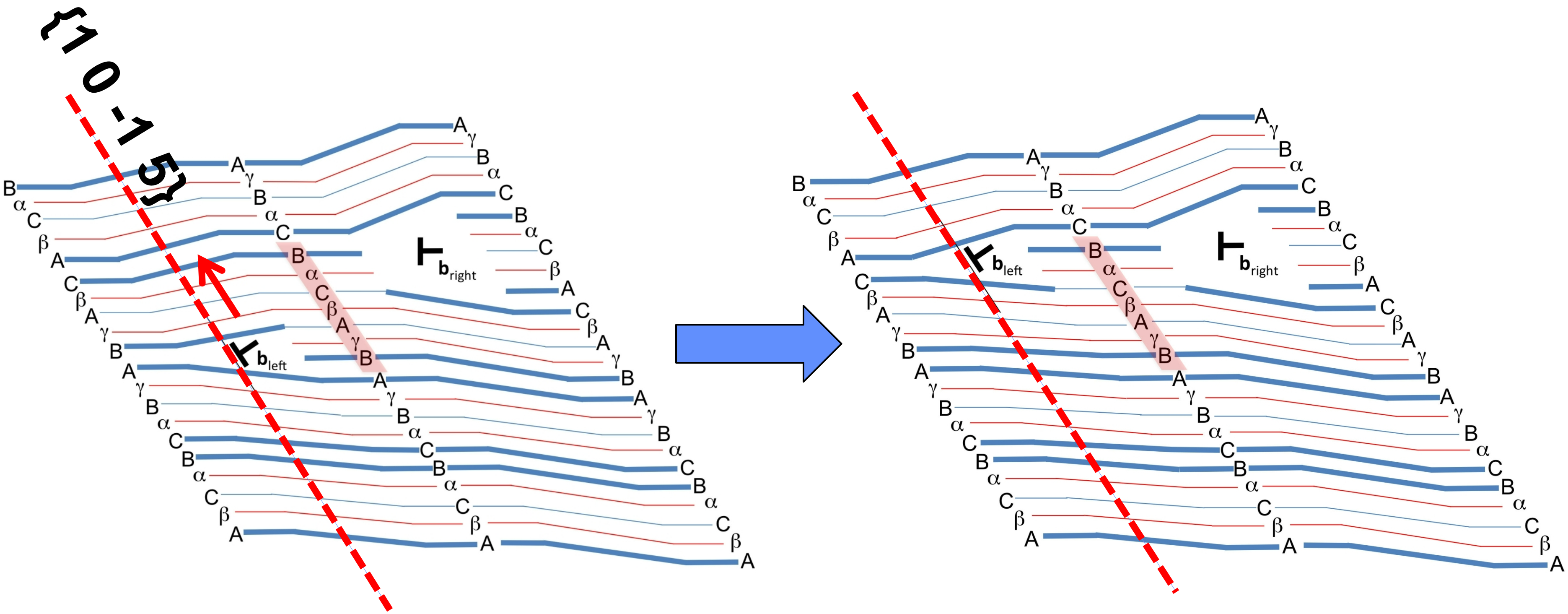
Medlin, Erickson, Limmer, Yelton, Siegal, J. Mat. Sci. 2014

Core can re-configure via glide of the left partial dislocation on {1 0 -1 5} plane



-{1 0 -1 5} is densely packed plane in tetradymite structure
-Analogous to {001} plane in rock-salt structure.

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Conclusions

• We have investigated the core-structures of two types of dislocation in Bi_2Te_3.

(1/3)<2 -1 -1 0> (basal dislocation)

-Defect terminates at Te(1)-Te(1) layer, allowing for stoichiometric core.

-Weak dissociation on basal plane

(1/3)<0 -1 1 1> type dislocation

- Large Burgers vector component along the c-axis accommodates misorientations at low angle grain boundaries vicinal to (0001).

-Dissociated core structure:

Local 7-layer defect region consistent with single, septuple unit of Bi_3Te_4

Formation of partial dislocations is favorable from strain energy considerations.

7-layer defect provides a mechanism for accommodating tellurium deficiency.

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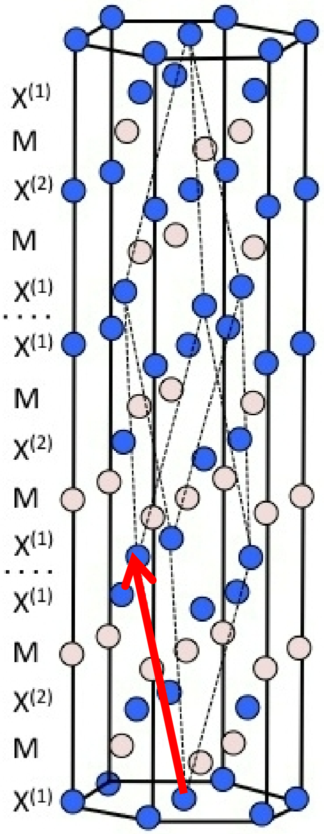
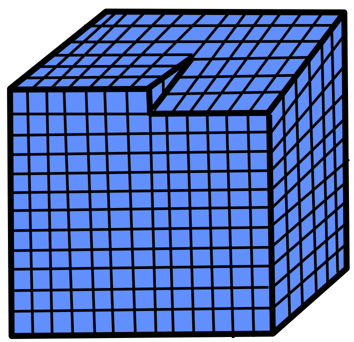
EXTRA

Non-basal dislocations:
Screw dislocations important to crystal growth

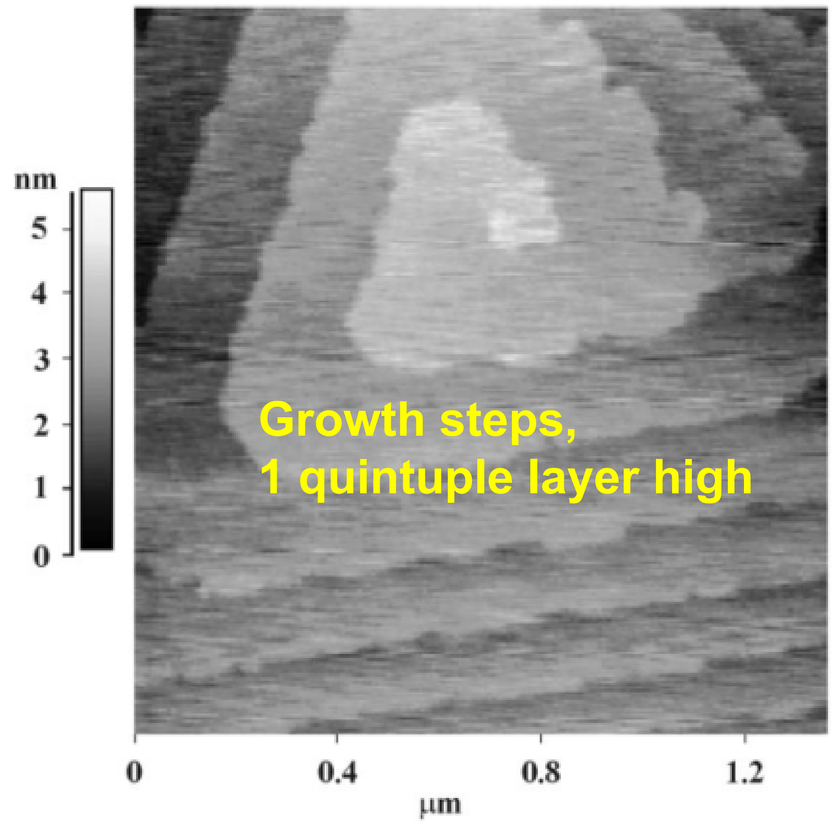


Screw Dislocation



$b = (1/3)[0\text{-}111)_H$
$= [001]_R$

Example: spiral growth steps at screw dislocation in Bi_2Te_3 thin film



M. Ferhat, J.C. Tedenac, J. Nagao, J. Crystal Growth (2000)

What about edge dislocations with non-basal Burgers vectors?

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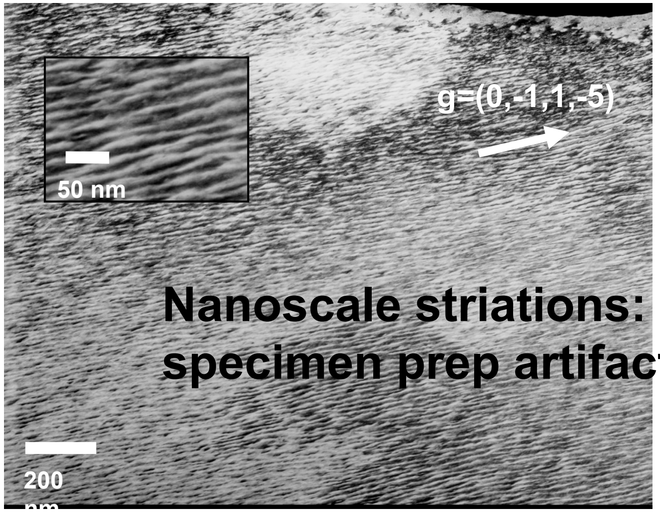
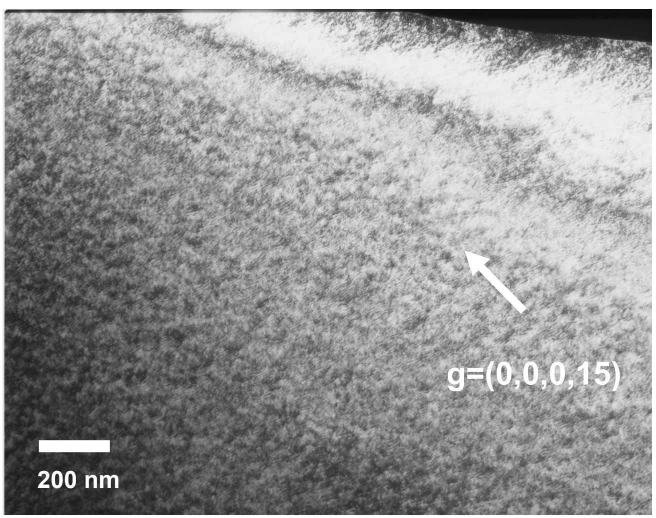
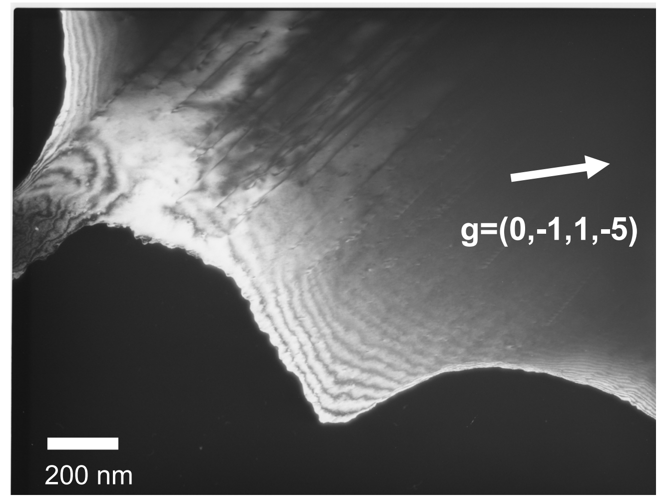
Aggressive ion-milling produces nanoscale artifacts in Bi_2Te_3

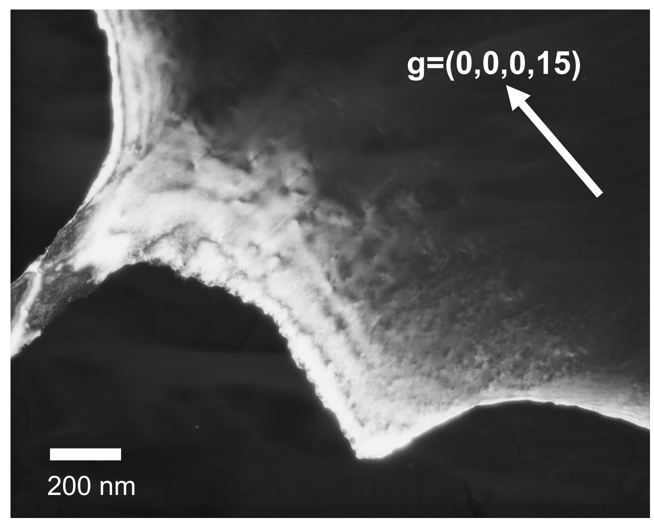
Ion Milled (Gatan DualMill 5 kV Ar+)





Electrochemical Polish





Can avoid artifacts using low-voltage, low-angle ion milling with cryo-cooling

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